Project Status Report

High End Computing Capability
Strategic Capabilities Assets Program

January 10, 2014

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Lou1 Users Transitioned to Lou parallel Data Migration Facility Archive System

- During a recent dedicated time, HECC systems engineers transitioned Lou1 users to the upgraded Lou parallel Data Migration Facility (pDMF) archive system.
- Users' files were migrated from an SGI Altix 4700 Itanium-based system to a backward-compatible x86-based system, enabling the Itanium system to be retired.
- All users can now easily transfer files between the Pleiades Lustre (nobackup) filesystems and Lou to simplify their archive workflow.
- Systems engineers also installed two front-end systems (for a total of four) to provide additional interactive access capability for users.
- The pDMF architecture provides users with a high-availability, high-performance system on a scalable platform that can grow with the agency's increasing archival requirements.

Mission Impact: HECC's parallel Data Migration Facility architecture provides a high-availability, scalable archive environment for NASA users.

HECC's Lou parallel Data Migration Facility archive system writes an average of about 2 petabytes of data per month to the tape libraries.

POCs: Bob Ciotti, bob.ciotti@nasa.gov, (650) 604-4408, NASA Advanced Supercomputing Division; Davin Chan, davin.chan@nasa.gov, (650) 604-3613, NASA Advanced Supercomputing Division, Computer Science Corp.

HECC Storage Resources Support Backup Data for Ames Information Technology Directorate

- NASA Ames Research Center's Information Technology Directorate (Code I) is now storing its system backup data on HECC's archive subsystem.
- HECC engineers worked with their counterparts in Code I to develop an optimal method to transfer and store up to 350 terabytes of data, utilizing the "Shift" high-speed automated file transfer tool developed by HECC staff.
- This collaborative solution leverages HECC's expertise and investment in archive storage, and reduces costs to the agency.
- Data is written to two redundant tape libraries located a kilometer apart on the Ames campus.
- HECC's archive infrastructure has the capacity to store up to 115 petabytes of data across six tape libraries using LTO5 magnetic tape storage technology.

Mission Impact: Collaborative technology solutions such as this leverage HECC's expertise and investment in archive storage, and reduce costs to the agency.

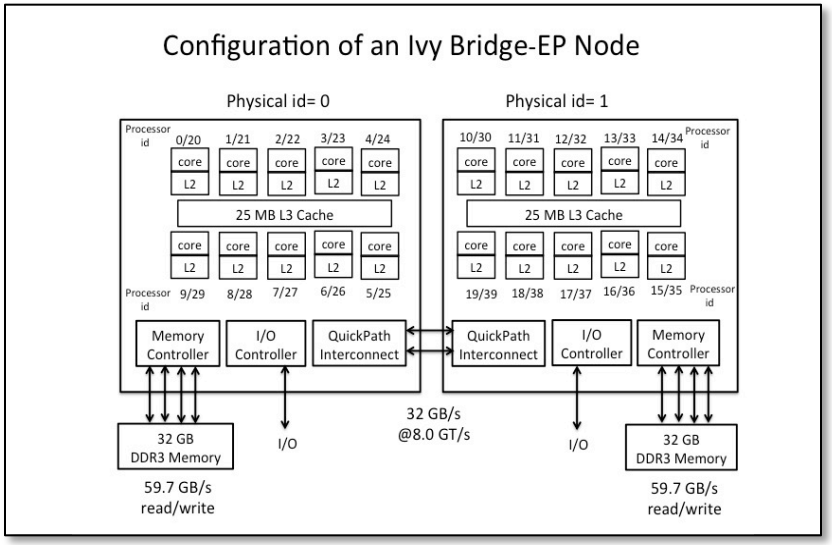
The HECC archive system currently stores about 65 petabytes of data across six tape libraries located at the main NASA Advanced Supercomputing (NAS) facility at Ames Research Center. A redundant tape library holds duplicate copies at a secondary NAS facility on the Ames campus.

POCs: Bob Ciotti, bob.ciotti@nasa.gov, (650) 604-4408, NASA Advanced Supercomputing Division; Davin Chan, davin.chan@nasa.gov, (650) 604-3613, NASA Advanced Supercomputing Division, Computer Science Corp.

Ivy Bridge Nodes Provide a Factor of Five Speedup over Endeavour for an OpenMP Code

- Recently, HECC Application Performance and Productivity (APP) team members observed that Endeavour user Alexander Lipatov (Goddard Space Flight Center) was running jobs on Pleiades Ivy Bridge nodes, and saw an opportunity for performance improvements through better node utilization techniques.
- Compared to Endeavor's Sandy Bridge nodes, the Ivy Bridge nodes have faster CPUs, better memory bandwidth, and substantially faster intra-node communication performance for applications that can fit into 20 cores.
- Lipatov's initial port of his OpenMP-based 3D hybrid code, used for Science Mission Directorate heliophysics modeling and simulation work, achieved a 3.5 times speedup over Endeavour.
- The APP team's investigation of the code performance showed that, because of script settings, the application was using only one socket. Another factor of 1.42 speedup was obtained with proper pinning of the OpenMP threads on both sockets—for an overall speed-up of 5.

Mission Impact: HECC expertise in application optimization regularly results in performance boosts and much faster turnaround time for scientists and engineers across all mission directorates.



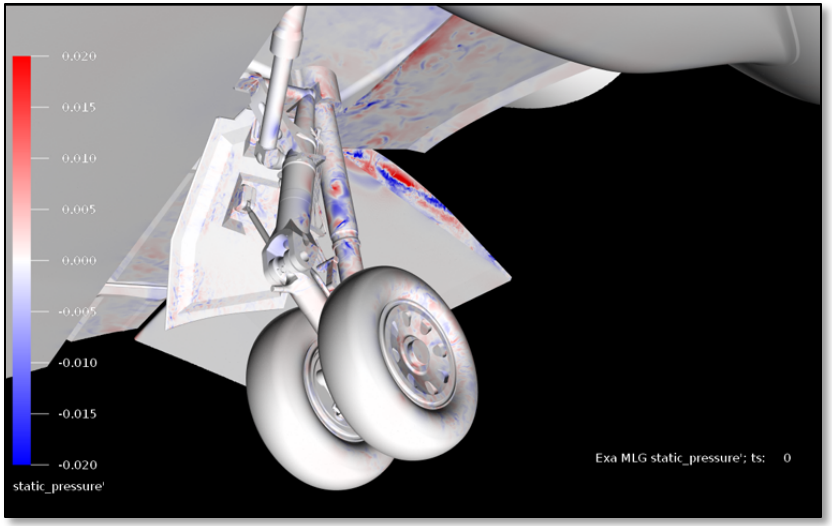
Configuration diagram of an Ivy Bridge node showing the Processor ID labeling for each core. For an OpenMP code run with 20 threads and a compact pinning of threads, all threads will be placed on the first socket labeled with Physical id=0. *(View in Slide Show mode and click image for full scale)*

POC: Johnny Chang, johnny.chang@nasa.gov, (650) 604-4356, NASA Advanced Supercomputing Division, Computer Sciences Corp.

Customized HECC Solution Enables More Accurate ARMD Simulations

- To support an Aeronautics Research Mission Directorate (ARMD) project, HECC systems experts upgraded the memory in four Pleiades Ivy Bridge nodes from 64 gigabytes (GB) to 256 GB.
- The project team (headed by Mehdi Khorrami, NASA Langley Research Center) uses Pleiades to analyze airframe noise generated by wing flaps and the main landing gear of a Gulfstream aircraft. The simulations capture the complex noise-producing aerodynamic mechanisms associated with these airframe components.
- The additional memory, procured by ARMD, allows project users to extend their flowfield simulation using the geometry of a full-scale aircraft. This improves the simulation accuracy and will help NASA to develop and refine advanced noise-reduction technologies for aircraft designs.

Mission Impact: HECC's onsite systems expertise enables prompt responses to requests for tailor-made resources that help NASA scientists stay at the forefront of their research fields.



Visualization of the simulated flow field for a Gulfstream aircraft in landing configuration, depicting surface pressures resulting from complex, unsteady flow interactions. This image shows the surface pressure field as affected by the presence of the main landing gear. Ehab Fares, Exa Corporation; Patrick Moran, NASA/Ames

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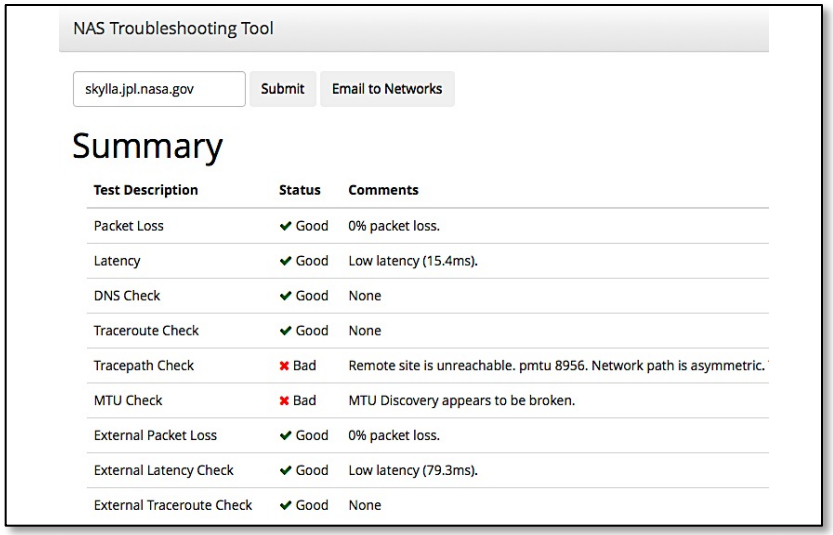
Network Team Develops Robust Automated Connectivity Troubleshooting Tool

- Utilizing a new HECC-developed tool, analysts can now identify a network problem in real time by entering the hostname or IP address of a remote system when a user calls in an issue. The tool can identify issues such as:
  - Whether a remote system has been blocked automatically by an HECC security manager tool.
  - Excessive packet loss, asymmetric routes, and high latency.
  - Domain Name System (DNS) resolution failure and network path maximum transmission unit (MTU) discovery failure.
  - Whether the problem originates within the NAS facility, NASA wide area network, or the Internet.
- The tool also connects to back-end flow capture tools and provides information about the maximum throughput rate and packet loss for a remote system.
- Future upgrades will include two-factor authentication, allowing users to directly access the tool.

Mission Impact: By developing specialized tools, HECC support staff can pinpoint and resolve network problems much more quickly and easily, enabling agency users to optimize time-to-solution performance.



Test Description	Status	Comments
Packet Loss	✔ Good	0% packet loss.
Latency	✔ Good	Low latency (15.4ms).
DNS Check	✔ Good	None
Traceroute Check	✔ Good	None
Tracepath Check	✖ Bad	Remote site is unreachable. pmtu 8956. Network path is asymmetric.
MTU Check	✖ Bad	MTU Discovery appears to be broken.
External Packet Loss	✔ Good	0% packet loss.
External Latency Check	✔ Good	Low latency (79.3ms).
External Traceroute Check	✔ Good	None

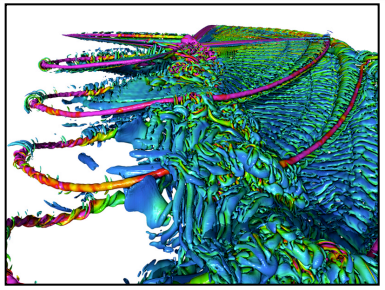
Results delivered by the new network troubleshooting tool during a test from a NAS facility network to a system at the Jet Propulsion Lab. Issues are flagged in red.

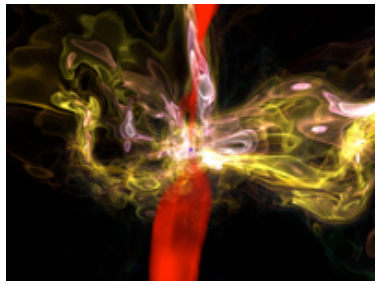
POC: Nichole Boscia, nichole.k.boscia@nasa.gov, (650) 604-0891, NASA Advanced Supercomputing Division, Computer Sciences Corp.

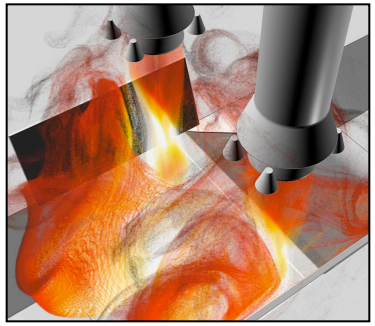
December Usage on Pleiades Exceeds 10.7 Million SBUs and Sets New Record

- December showed record-high usage of the Pleiades supercomputer, with 10.74 million Standard Billing Units (SBUs) used by NASA's science and engineering organizations, exceeding the previous record of 9.37 million SBUs (set in September 2013) by over 14%.
- This increase was enabled by the addition of 3,312 Ivy Bridge nodes in August and by efficient operations that delivered better than 97% availability.
- The top project in each Mission Directorate each used over 600,000 SBUs and together accounted for 20% of the usage.
- The next 12 projects each used over 200,000 SBUs, and together accounted for another 32% of the total usage.
- Pleiades will be expanded during the second quarter of FY14 to continue to address the requirements of NASA's users.

Mission Impact: Increasing Pleiades' system capacity provides Mission Directorates with more resources for the accomplishment of their goals and objectives.







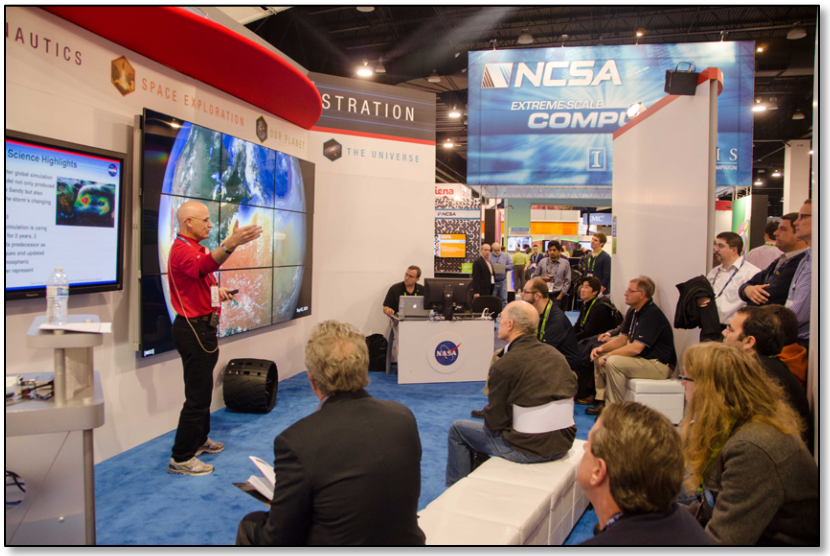
Images representing projects that were among the top users of computer time in their respective Mission Directorates. Clockwise from top: 1) Aft view of the UH-60 helicopter rotor detached eddy simulation, ARMD, N. Chaderjian; 2) Simulation showing time-accurate particle traces colored by temperature below Solid Rocket Booster nozzles, HEOMD, C. Kiris & J. Housman; 3) Density volume rendering of an isolated, magnetized, supersonically-turbulent core 20,000 years after the formation of the central high-mass protostar, SMD, A. Cunningham & A. T. Myers.

POC: Catherine Schulbach, catherine.h.schulbach@nasa.gov, (650) 604-3180, NASA Advanced Supercomputing Division

New Mac Mini Cluster Provides Improved Reliability to HECC Traveling Hyperwall

- HECC visualization system experts recently upgraded the eight-year-old cluster that drove the smaller, traveling version of the hyperwall-2 visualization system.
  - System reliability is critical to support high-visibility presentations on the hyperwall at the annual "SC" supercomputing conference and other events.
  - The reliability of the aging cluster was uncertain, and any needed repairs would be difficult and time-consuming. The previous cluster was also heavy, making it difficult to move and maneuver.
- The team designed and built a replacement cluster with Mac Minis, which have higher performance than the old system, weigh dramatically less, and are easier to replace.
- The system was completed and software and demonstration materials were installed in time for the SC13 conference, despite the upgrade window being reduced by 50% due to the federal shutdown.

Mission Impact: HECC's robust, portable hyperwall cluster provides critical reliability to visual demonstrations that showcase NASA's science and engineering advances across all mission directorates, at important conferences and other public events.



Phil Webster, Chief of the Computational and Information Science and Technology Office at NASA's Goddard Space Flight Center, points out results of a global climate simulation presented on the traveling hyperwall at the SC13 conference, held in Denver in November 2013.

POCs: David Ellsworth, david.ellsworth@nasa.gov, (650) 604-0721, NASA Advanced Supercomputing Division, Computer Sciences Corp; Chris Henze, chris.henze@nasa.gov, (650) 604-3959, NASA Advanced Supercomputing Division

Understanding Earth's Evolving Ocean, Ice, Carbon, and Ecology *

- As part of the Consortium for Estimating the Circulation and Climate of the Ocean (ECCO), a research team at the Jet Propulsion Laboratory and Massachusetts Institute of Technology is running numerical ocean simulations and data assimilation codes on Pleiades to produce quantitative reconstructions of the time-evolving global ocean state.
- These ECCO reconstructions are being used for numerous applications, for example to:
  - Study the impact of ocean currents on glacier acceleration around Greenland and Antarctica.
  - Simulate the role of the ocean in the global carbon cycle.
  - Drive ocean ecology and fishery models.
- Access to Pleiades allows the ECCO team to solve these massive numerical ocean simulation and minimization problems.

Mission Impact: Enabled by HECC resources, numerical reconstructions of the time-evolving global ocean state help improve our understanding of the ocean's role in observed climate variability and our predictions of future climate change scenarios.

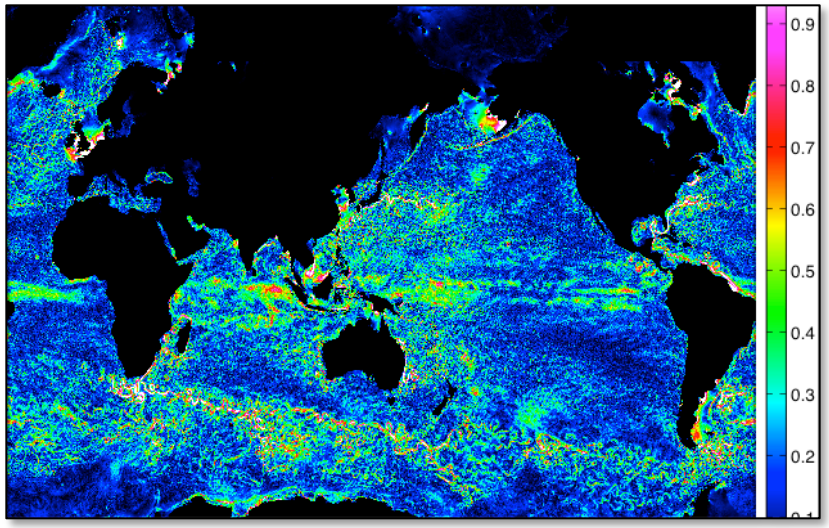


Image from a simulation showing ocean depth. Using computationally intensive models, together with remotely sensed and in situ data, is the only way we know to truly see how the planet is evolving globally in a consistent and comprehensive way. *Christopher Henze, Bron Nelson, NASA/Ames*

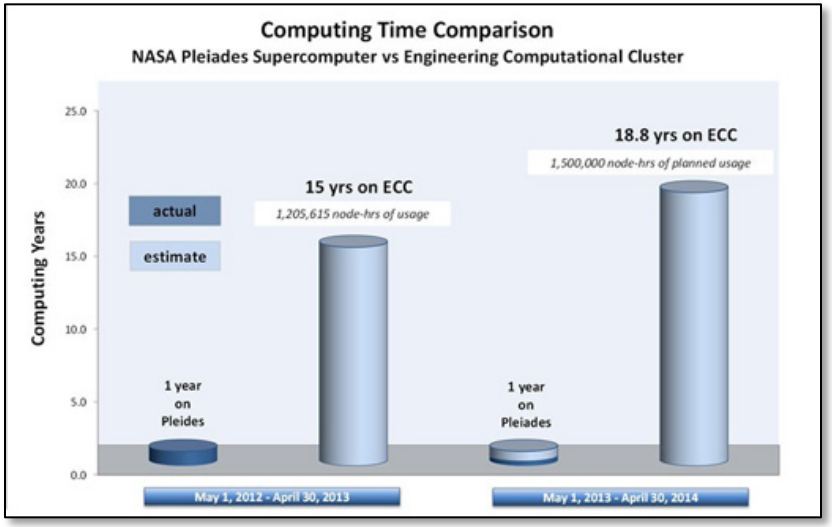
POCs: Christopher Hill, cnh@mit.edu, Massachusetts Institute of Technology; Dimitris Menemenlis, (818) 354-1656, menemenlis@jpl.nasa.gov, Jet Propulsion Laboratory

** HECC provided supercomputing resources and services in support of this work*

Simulations for International Space Station (ISS) Loads Analysis *

- A team at NASA Johnson Space Center (JSC) ran comprehensive structural load simulations on Pleiades to extend the life of the ISS to 2020 and beyond. Work included:
  - Analyses to determine parameters for ISS attitude control maneuvers for the new flight software version.
  - Solar Array Keep-Out-Zone calculations for ISS maneuvers, reboosts, and visiting vehicle proximity operations.
  - Verification Loads Analysis for the SpaceX-2, H-II Transfer Vehicle 4, and Orbital Demo 1 missions.
  - Special studies for the Stratospheric Aerosol and Gas Experiment 3 (SAGE-3) and Multiple User System for Earth Sensing (MUSES) payloads.
- Pleiades enabled the JSC team to complete these simulations for an ISS milestone—a task that would take several years on JSC's Engineering Computational Cluster.

Mission Impact: The Pleiades supercomputer's capability and capacity enabled the timely completion of structural loads analyses that led to lower operational risks and constraints for the International Space Station.



Use of NASA's Pleiades supercomputer greatly decreased the time required to run tens of thousands of loads simulations required for each of multiple missions to the ISS. *(View in Slide Show mode and click image for full scale)*

POC: Michael Grygier, michael.s.grygier@nasa.gov, (281) 483-6398, NASA Johnson Space Center

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HECC Facility Hosts Several Visitors and Tours in December 2013

- HECC hosted 7 tour groups in December; guests learned about the agency-wide missions being supported by Pleiades, and viewed scientific results on the hyperwall system. Visitors this month included:
  - John Holdren, Director of the White House Office of Science and Technology Policy (OSTP), and Rick Weiss, Assistant Director of OSTP, who met with senior staff at Ames Research Center (ARC). Both received an overview of HECC Project resources and services and their impact on NASA science and engineering missions, and a tour of the quantum computer room.
  - International partners from the Solar System Exploration Research Virtual Institute, who held their annual executive meeting at ARC, and groups from the Republic of Korea Information and Communication Technology Policy and the King Abdulaziz City for Science & Technology, who met with NAS staff. Both groups received a tour of the NAS facility, including the quantum computer room.

HECC Project Manager Rupak Biswas (far right) gave an overview of the project's resources and services to John Holdren (seated at center), Assistant to the President for Science and Technology and Director of the White House Office of Science and Technology Policy.

POC: Gina Morello, gina.f.morello@nasa.gov, (650) 604-4462, NASA Advanced Supercomputing Division

Papers and Presentations

- "**Ocean-Driven Heating of Europa's Icy Shell at Low Latitudes**," K. M. Soderlund, B. E. Schmidt, J. Wicht, D. D. Blankenship, Nature Geosciences: Letters (2013), December 1, 2013. *
  http://www.nature.com/ngeo/journal/vaop/ncurrent/full/ngeo2021.html
- "**Analyzing Tropical Waves Using the Parallel Ensemble Empirical Model Decomposition Method: Preliminary Results from Hurricane Sandy**," B.-W. Shen, S. Chueng, J.-L. F. Li, Y.-L. Wu, Earthzine (as part of the 2013 Earth Science Technology Showcase), December 2, 2013. *
  http://www.earthzine.org/2013/12/02/analyzing-tropical-waves-using-the-parallel-ensemble-empirical-model-decomposition-method-preliminary-results-from-hurricane-sandy/?shareadraft=baba578724_529ced40a0018
- "**Simulations and Visualizations of Hurricane Sandy (2012) as Revealed by the NASA CAMVis**," B.-W. Shen, Earthzine (as part of the 2013 Earth Science Technology Showcase), December 2, 2013. *
  http://www.earthzine.org/2013/12/02/simulations-and-visualizations-of-hurricane-sandy-2012-as-revealed-by-the-nasa-camvis/?shareadraft=baba578799_529cfef9aa937
- "**Constrained Simulation of the Bullet Cluster**," C. Lage, G. Farrar, arXiv:1312.0959 [astro-ph.CO], December 3, 2013. *
  http://arxiv.org/abs/1312.0959

** HECC provided supercomputing resources and services in support of this work*

Papers and Presentations (cont.)

- "**Constraints on Diffuse Gamma-Ray Emission from Structure Formation Processes in the Coma Cluster**," F. Zandanel, S. Ando, arXiv:1312.1493 [astro-ph.HE], December 5, 2013. *
  http://arxiv.org/abs/1312.1493
- **2013 American Geophysical Union**, San Francisco, CA, December 9-13, 2013.
  - "**Mechanism, Dynamics and Evolution of Small-Scale Dynamo on the Sun**," I. Kitiashvili, A. Kosovichev, N. Mansour, A. Wray. *
  - "**Approach to Integrate Global-Sun Models of Magnetic Flux Emergence and Transport for Space Weather Studies**," N. Mansour, A. Wray, P. Mehrotra, C. Arge, C. Henney, W. Manchester, H. Godinez, J. Koller, A. Kosovichev, P. Scherrer, J. Zhao, B. Stein, T. Duvall, Y. Fan. *
  - "**Parallelization of the Ensemble Empirical Model Decomposition (PEEMD) Method on Multi- and Many-core Processors**," S. Cheung, B.-W. Shen, J. F. Li, P. Mehrotra. *
  - "**Multiscale Processes of Hurricane Sandy (2012) as Revealed by the CAMVis-MAP**," B.-W. Shen, J.-L. F. Li, S. Cheung. *
  - "**HECC: Meeting NASA's High-End Computing Goals Through Innovation**," W. Thigpen.
  - "**Intercomparisons of Prognostic, Diagnostic, and Inversion Modeling Approaches for Estimation of Net Ecosystem Exchange over the Pacific Northwest Region**," D. P. Turner, A. R. Jacobson, R. R. Nemani. *
  - "**Fertilization: What Models Can Talk to Observations**," W. Wang, R. R. Nemani, K. M. Schaefer, C. R. Schwalm, D. N. Huntzinger, G. Zhang, J. Xiong. *

** HECC provided supercomputing resources and services in support of this work*

Papers and Presentations (cont.)

- **2013 American Geophysical Union** (cont.)
  - "**Trend in Surface-Water Balance over the Western United States from Downscaled CMIP5 Climate Projections**," J. Xiong, W. Wang, F. S. Melton, C. Milesi, R. R. Nemani. *
  - "**Knowledge Acquisition and Management for the NASA Earth Exchange (NEX)**," P. Votava, A. Michaelis, R. R. Nemani. *
  - "**Global Web-Enabled Landsat Data**," D. P. Roy, V. Kovalskyy, I. Kommareddy, P. Votava, R. R. Nemani, A. Egorov, M. Hansen, L. Yan. *
  - "**U.S. Forest Disturbance Rates Observed from Landsat**," C. Huang, S. N. K. Schleeweis, F. Zhao, M. Lindsey, J. Masek, W. B. Cohen, G. G. Moisen, R. R. Nemani. *
  - "**Satellite Mapping of Agricultural Water Requirements in California**," F. S. Melton, C. Lund, L. Johnson, A. Guzman, S. Hiatt, K. Post, D. Adhikari, C. Rosevelt, S. Keefauver, G. Miller, A. Michaelis, P. Votava, B. Temesgen, K. Frame, R. R. Nemani. *
  - "**Detecting Forest Disturbance Events from MODIS and Landsat Time Series for the Conterminous United States**," G. Zhang, S. Ganguly, S. S. Saatchi, S. C. Hagen, N. Harris, Y. Yu, R. R. Nemani. *
  - "**Satellite Measurements of Changes in Water Storage and Their Impact on Vegetation Dynamics**," H. Hashimoto, R. R. Nemani. *
  - "**Deriving Continuous Fields of Tree Cover at 1-m over the Continental United States From the National Agriculture Imagery Program (NAIP) Imagery to Reduce Uncertainties in Forest Carbon Stock Estimation**," S. Ganguly, S. Basu, S. Mukhopadhyay, A. Michaelis, C. Milesi, P. Votava, R. R. Nemani. *

** HECC provided supercomputing resources and services in support of this work*

Papers and Presentations (cont.)

- **2013 American Geophysical Union** (cont.)
  - "**A Model-Based Estimate of the Relative Importance of Climate Warming, CO2-Fertilization and Nitrogen Deposition to Global Terrestrial Carbon Uptake**," G. Bala, D. Narayanappa, R. Chaturvedi, K. Caldeira, R. R. Nemani. *
  - "**A Community-Driven Workflow Recommendations and Reuse Infrastructure**," J. Zhang, P. Votava, T. J. Lee, C. Lee, S. Xiao, R. R. Nemani, I. Foster.
- "**A High-Frequency Doppler Feature in the Power Spectra of Simulated GRMHD Black Hole Accretion Disks**," S. Wellons, Y. Zhu, D. Psaltis, R. Narayan, J. E. McClintock, arXiv:1312.3333 [astro-ph.HE], December 11, 2013. *
  http://arxiv.org/abs/1312.3333
- "**The Mutual Interaction Between Population III Stars and Self-Annihilating Dark Matter**," A. Stacy, A. H. Pawlik, V. Bromm, A. Loeb, arXiv:1312.3117 [astro-ph.CO], December 11, 2013. *
  http://arxiv.org/abs/1312.3117

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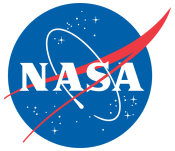
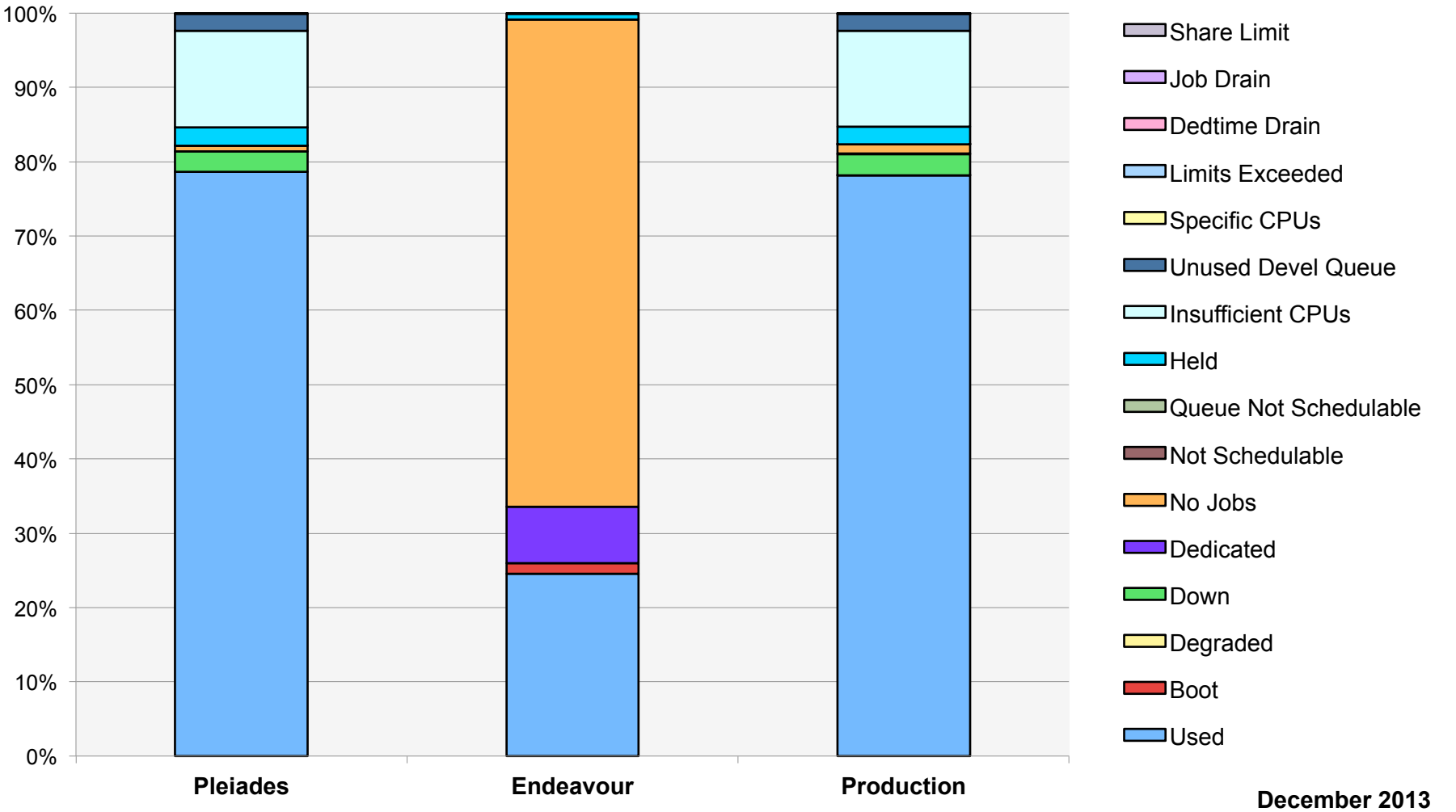
News and Events

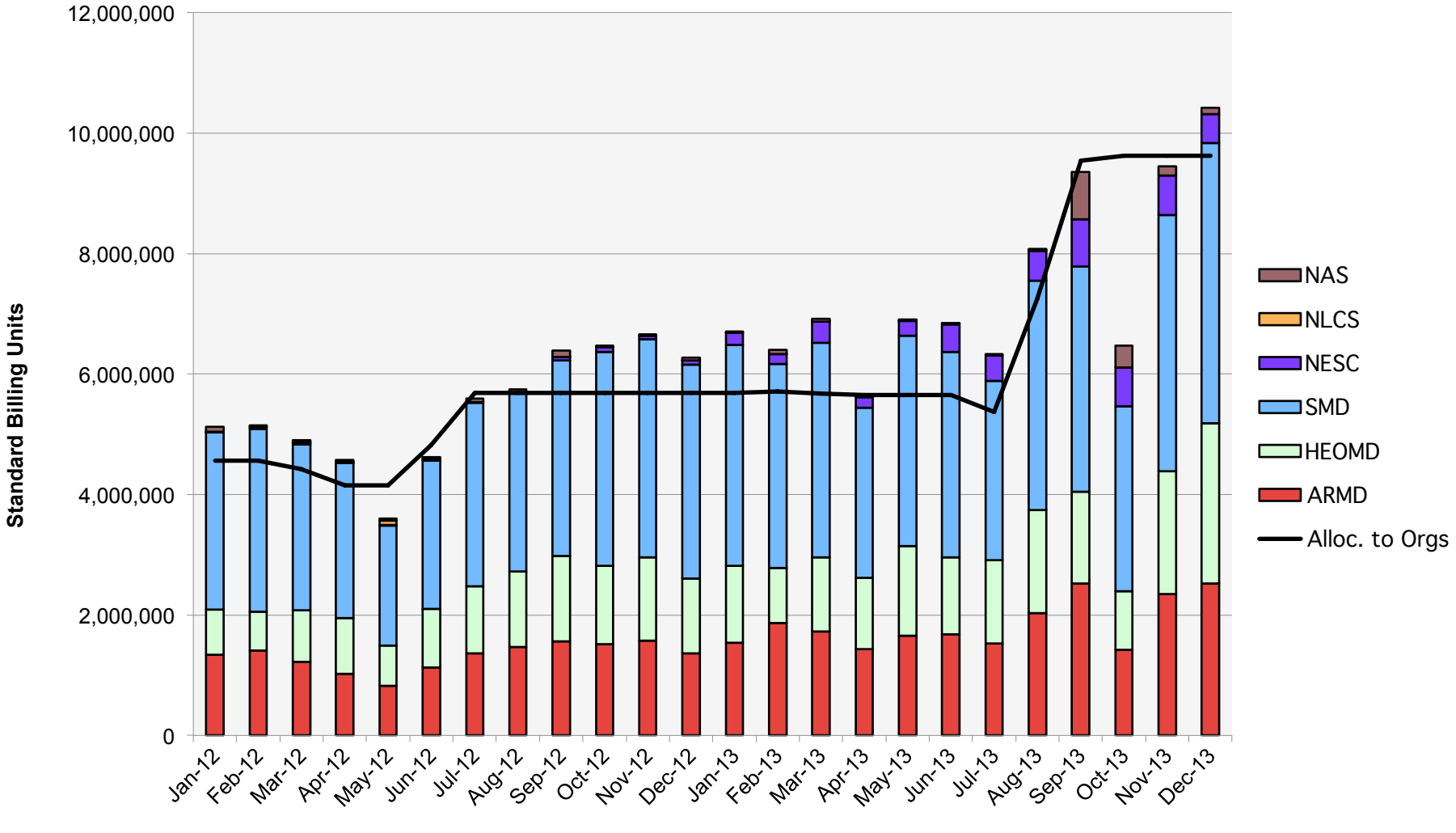


- **NASA's Rupak Biswas Investigates the Weird World of Quantum Computing**, *insideHPC,* December 2, 2013—insideHPC's John Kirkley interviews Rupak Biswas at the November SC13 conference, about the agency's involvement in the evolving world of quantum computing.
  http://insidehpc.com/2013/12/02/nasas-rupak-biswas-investigates-weird-world-quantum-computing/
- **NASA Moves Earth Science Tools, Platform to the Cloud**, *GCN.com,* December 16, 2013—NASA has partnered with Amazon Web Services to create OpenNEX, making terabytes of NASA Earth Exchange (NEX) climate and Earth science data available to researchers, app developers, academia, and the general public via the cloud.
  The Pleiades supercomputer is a key component of the NEX collaborative workspace.
  http://gcn.com/articles/2013/12/16/nasa-opennex.aspx

HECC Utilization



HECC Utilization Normalized to 30-Day Month



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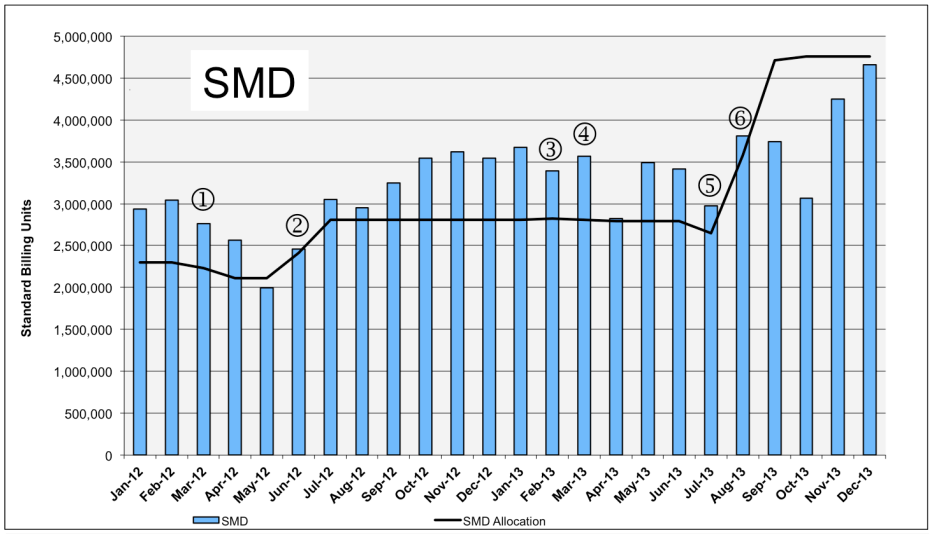
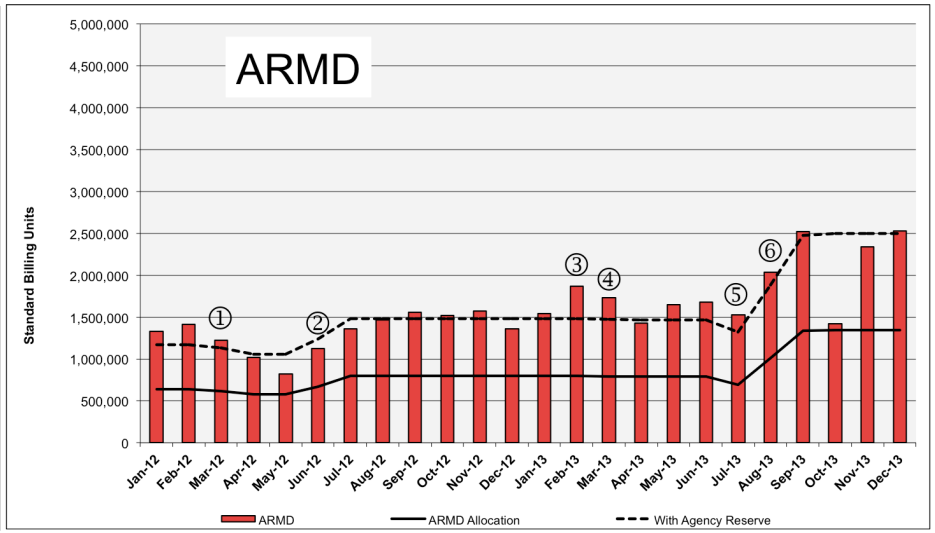
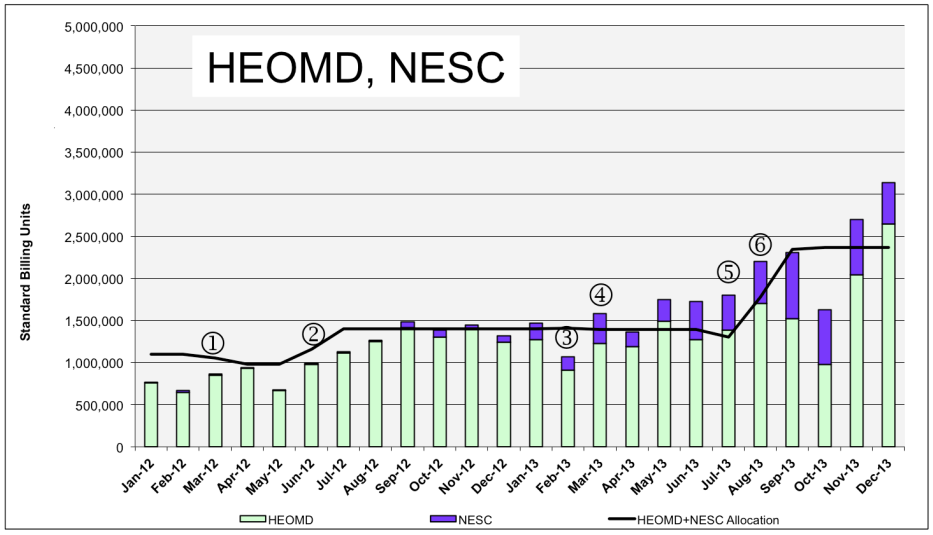






① 28 Harpertown Racks retired

② 24 Sandy Bridge Racks added

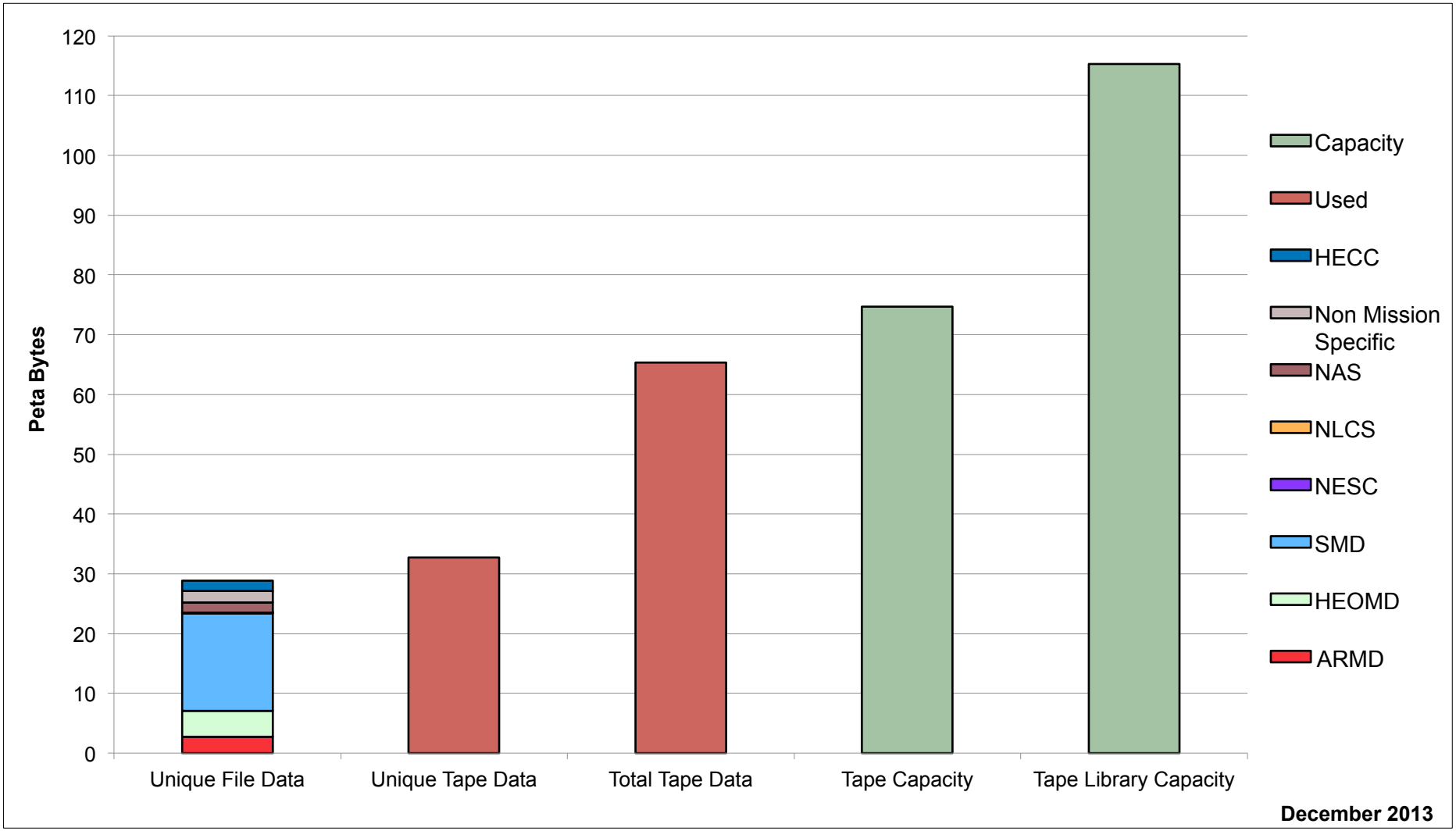
③ Columbia 21, 23, and 24 retired, Endeavour 2 added

④ Columbia 22 retired; Endeavour 1 added

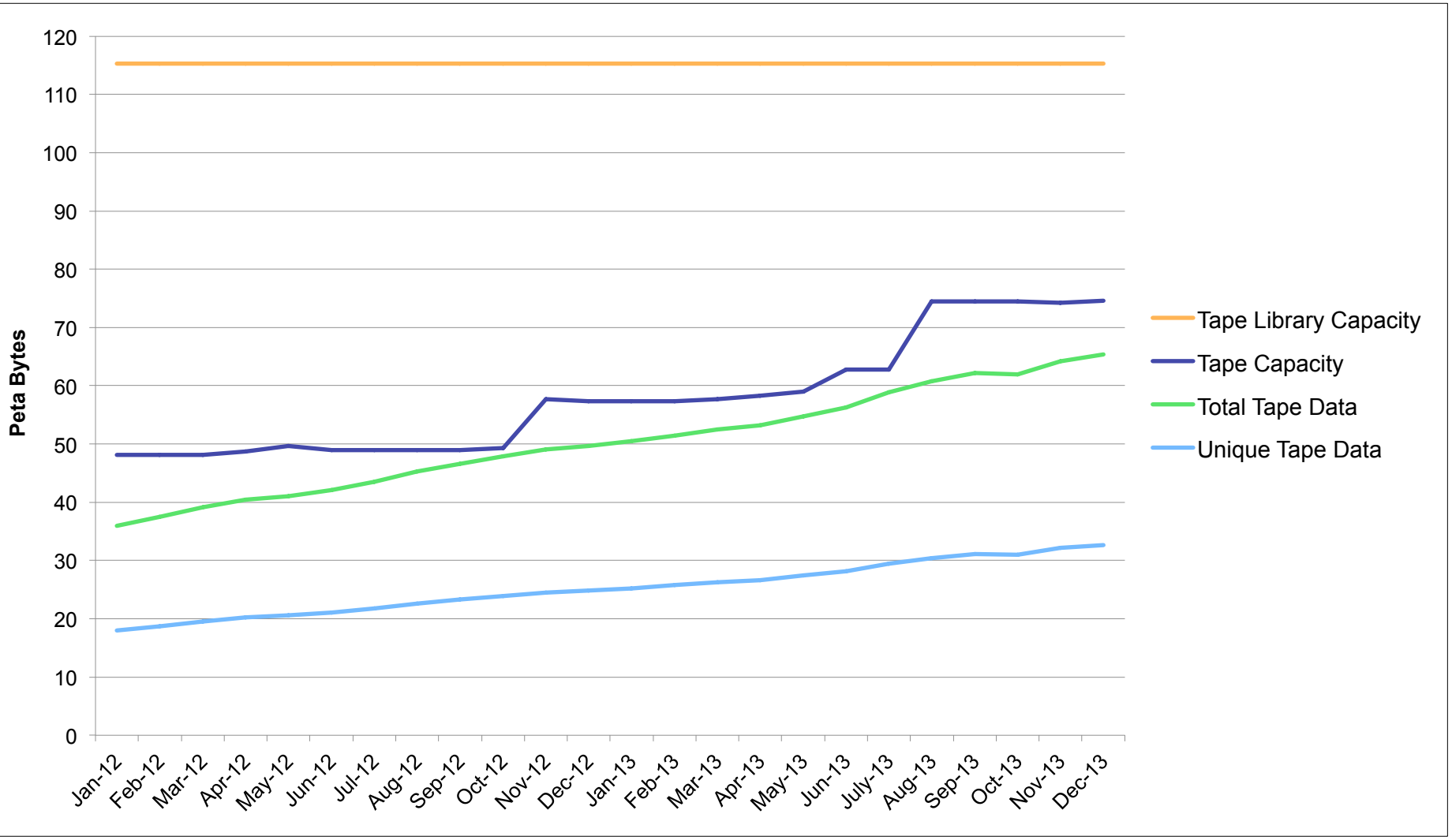
⑤ 32 Harpertown Racks retired

⑥ 32 Harpertown Racks retired; 46 Ivy Bridge Racks added

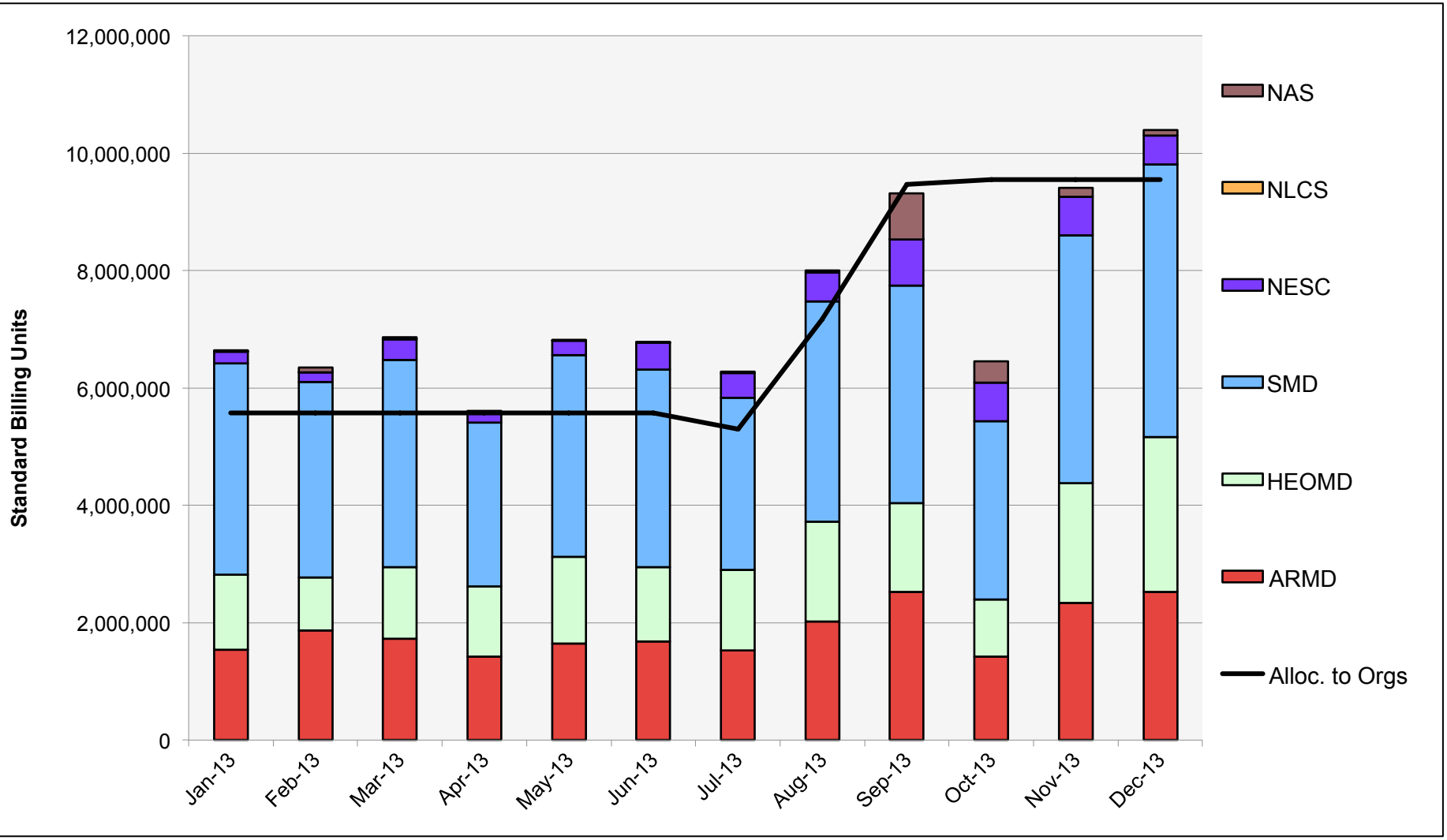
Tape Archive Status



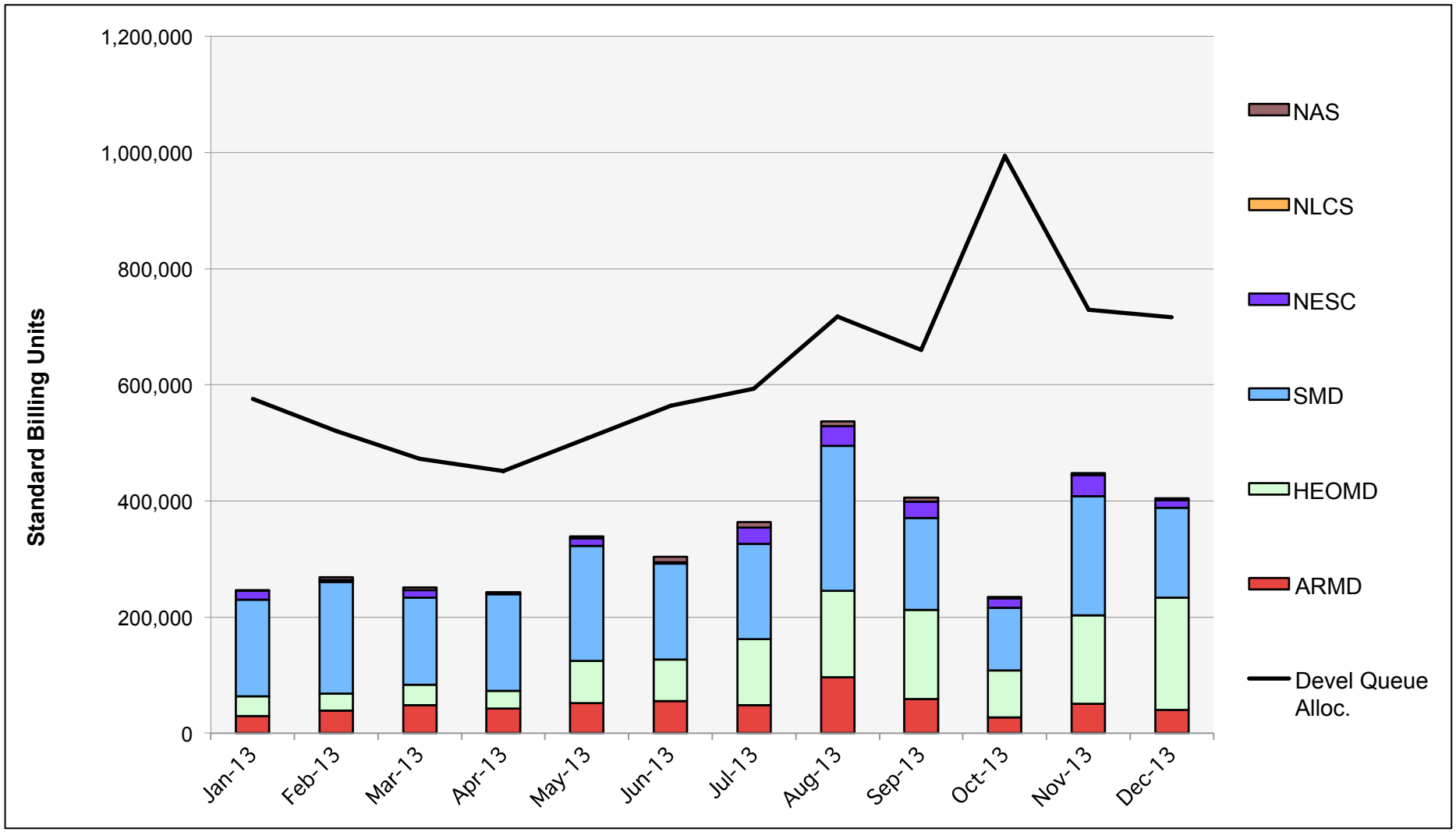
Tape Archive Status



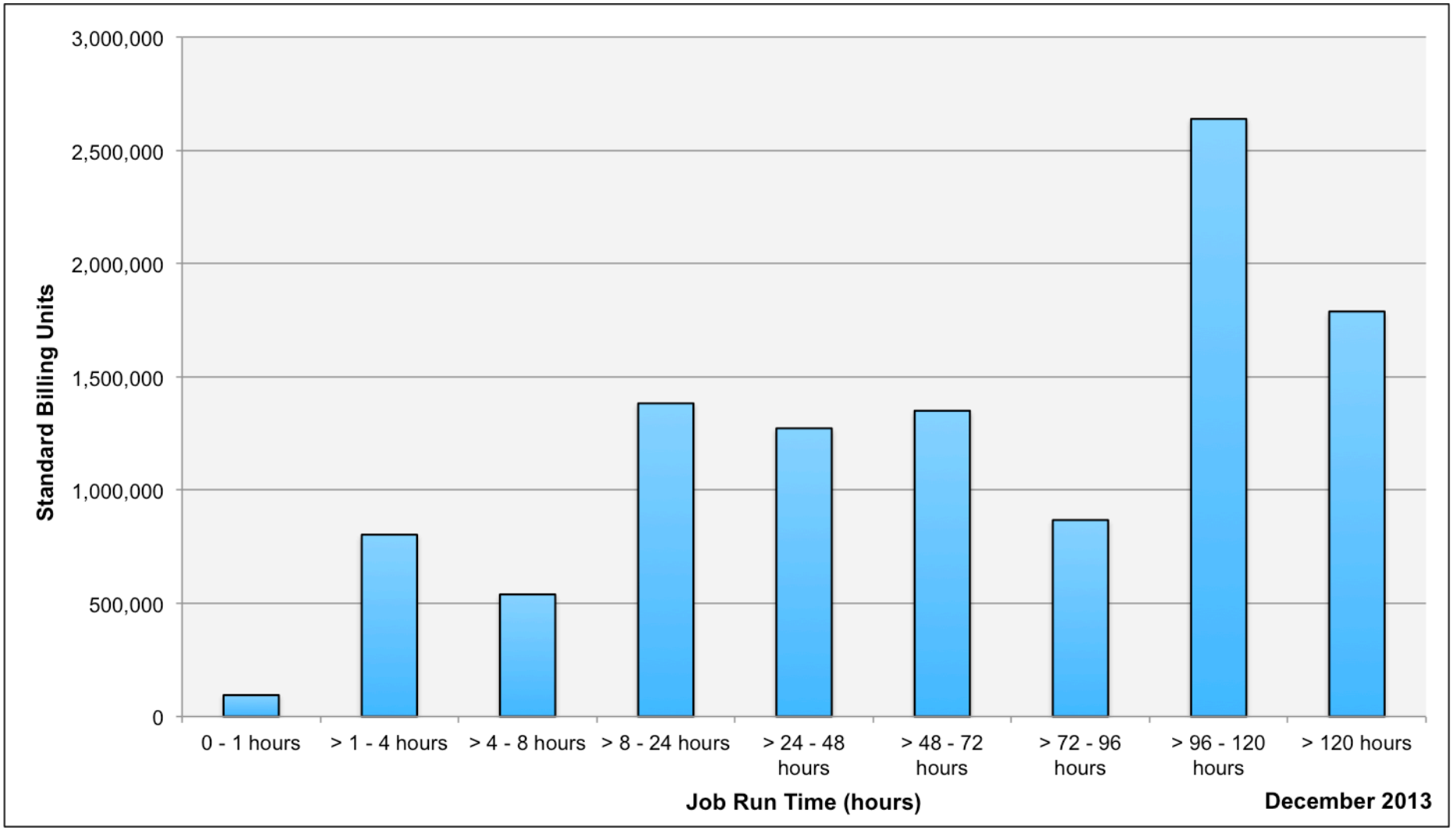
Pleiades:
SBUs Reported, Normalized to 30-Day Month



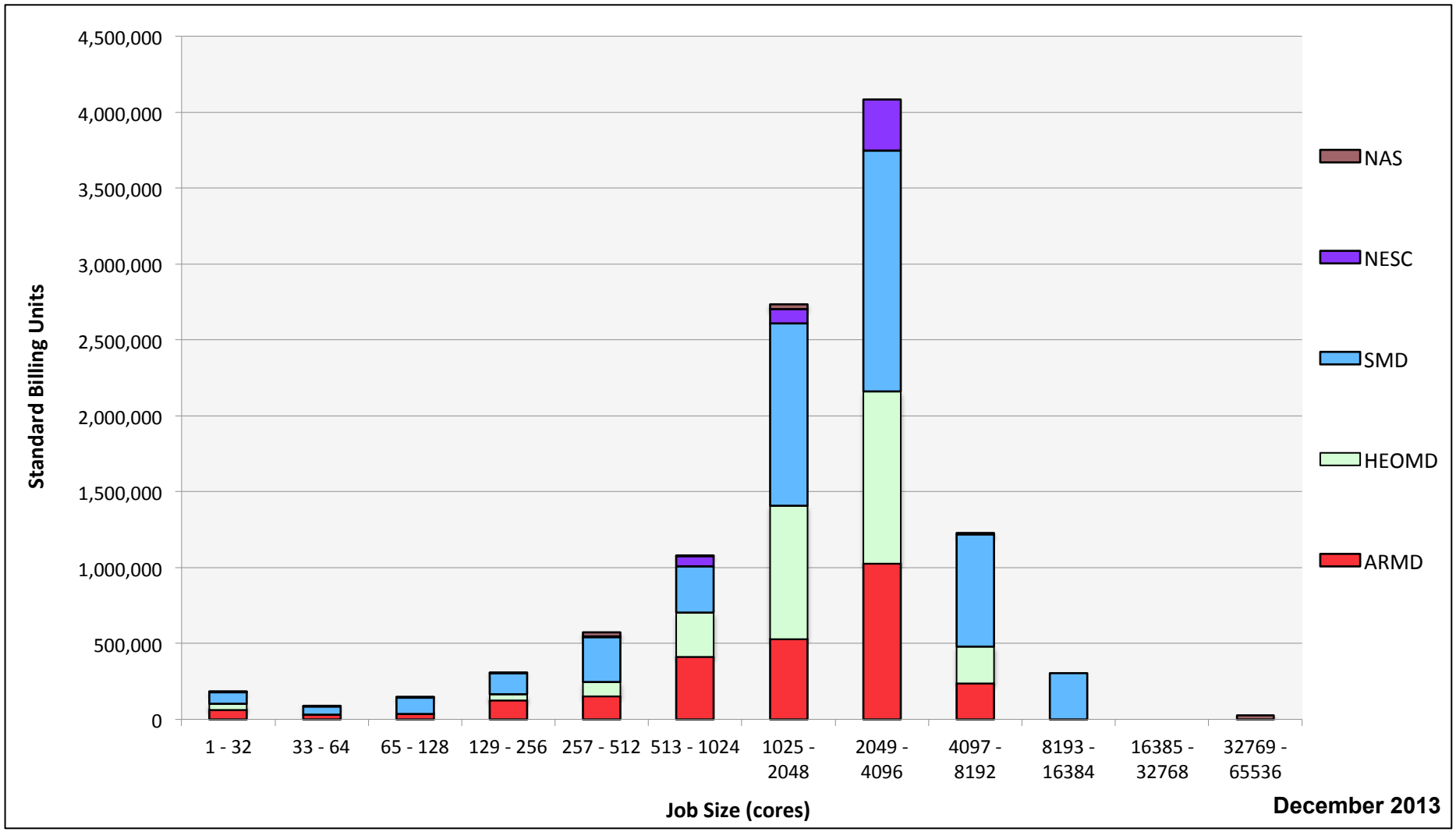
Pleiades:
Devel Queue Utilization



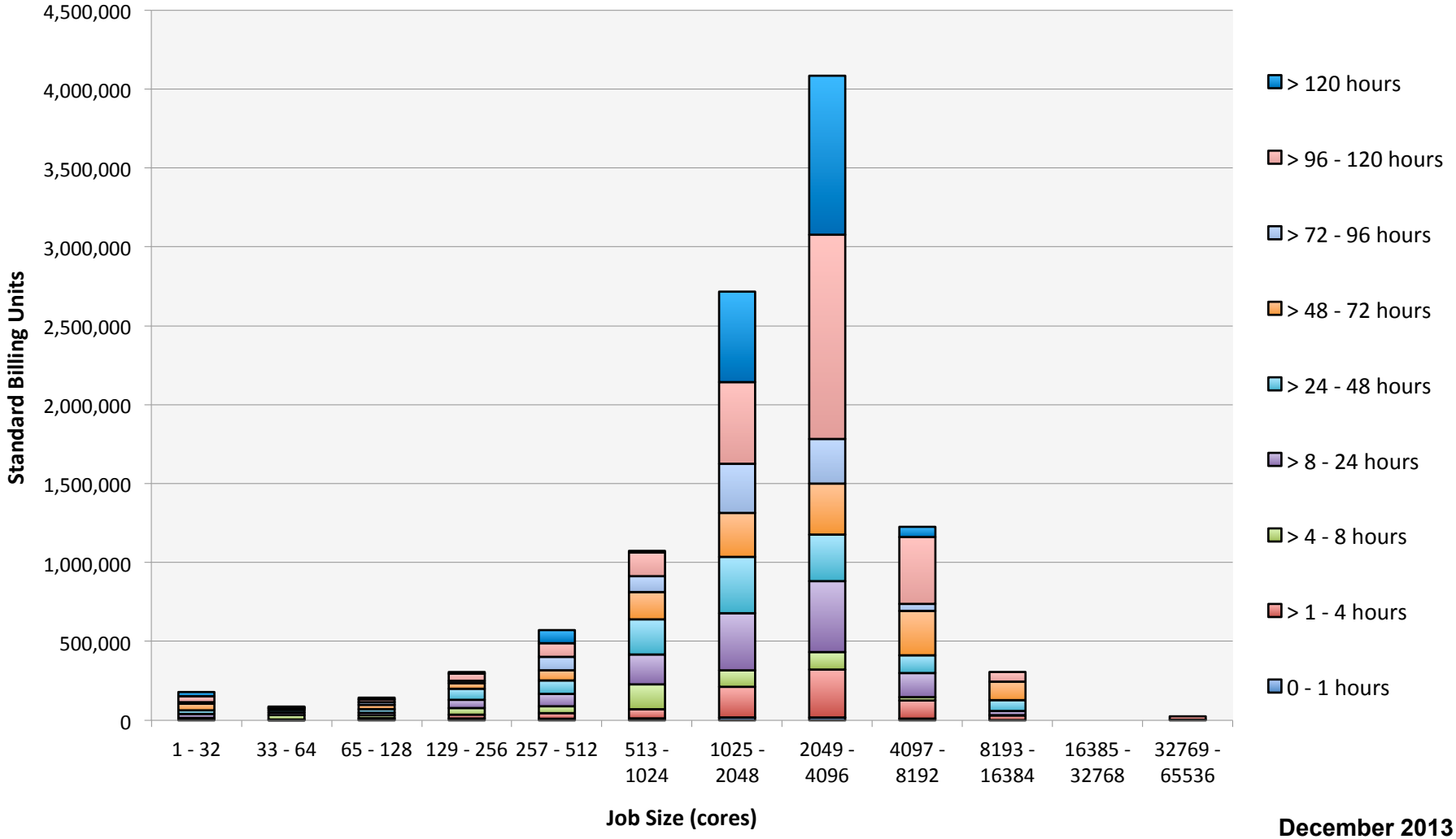
Pleiades:
Monthly Utilization by Job Length



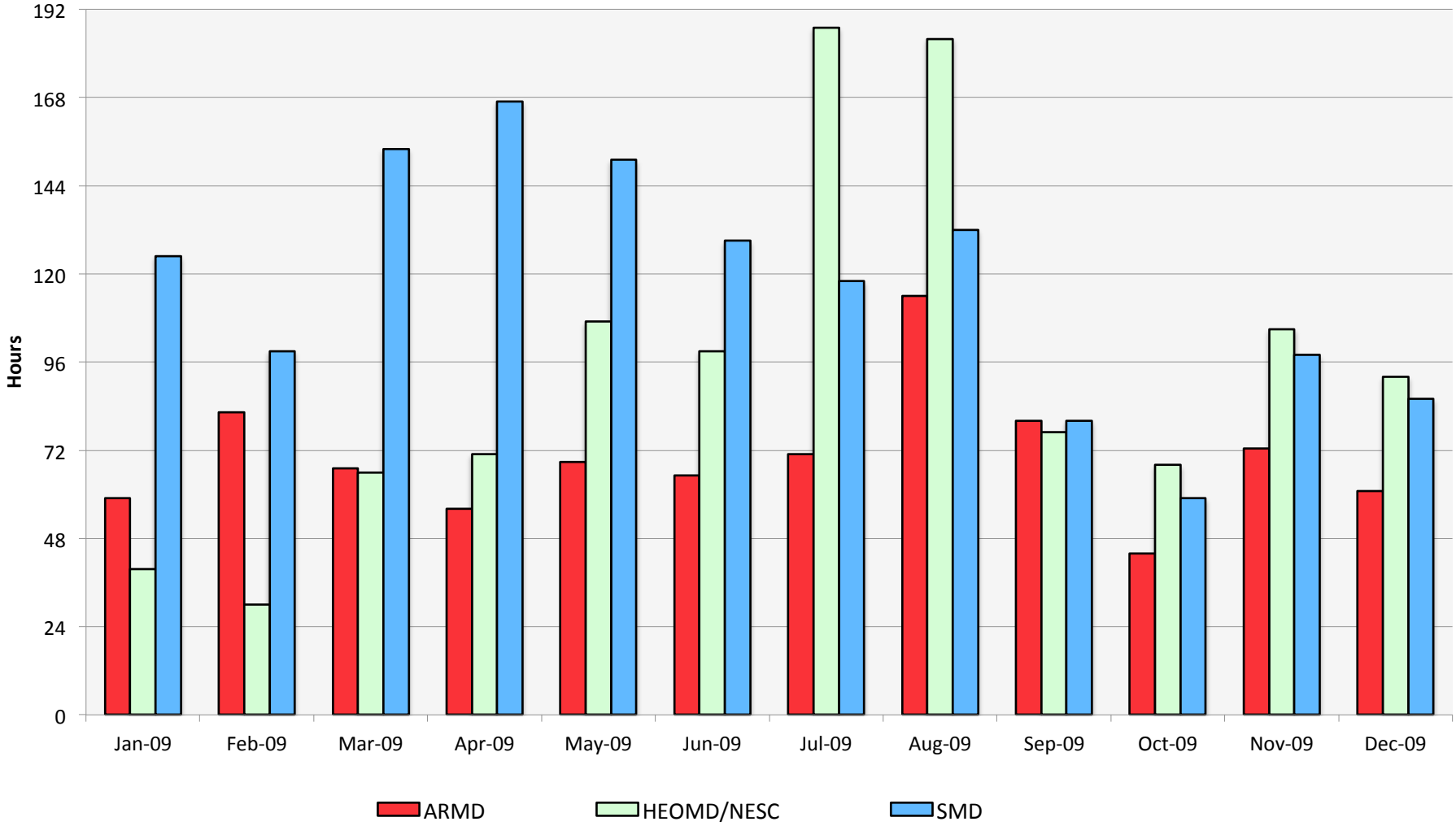
Pleiades:
Monthly Utilization by Size and Mission



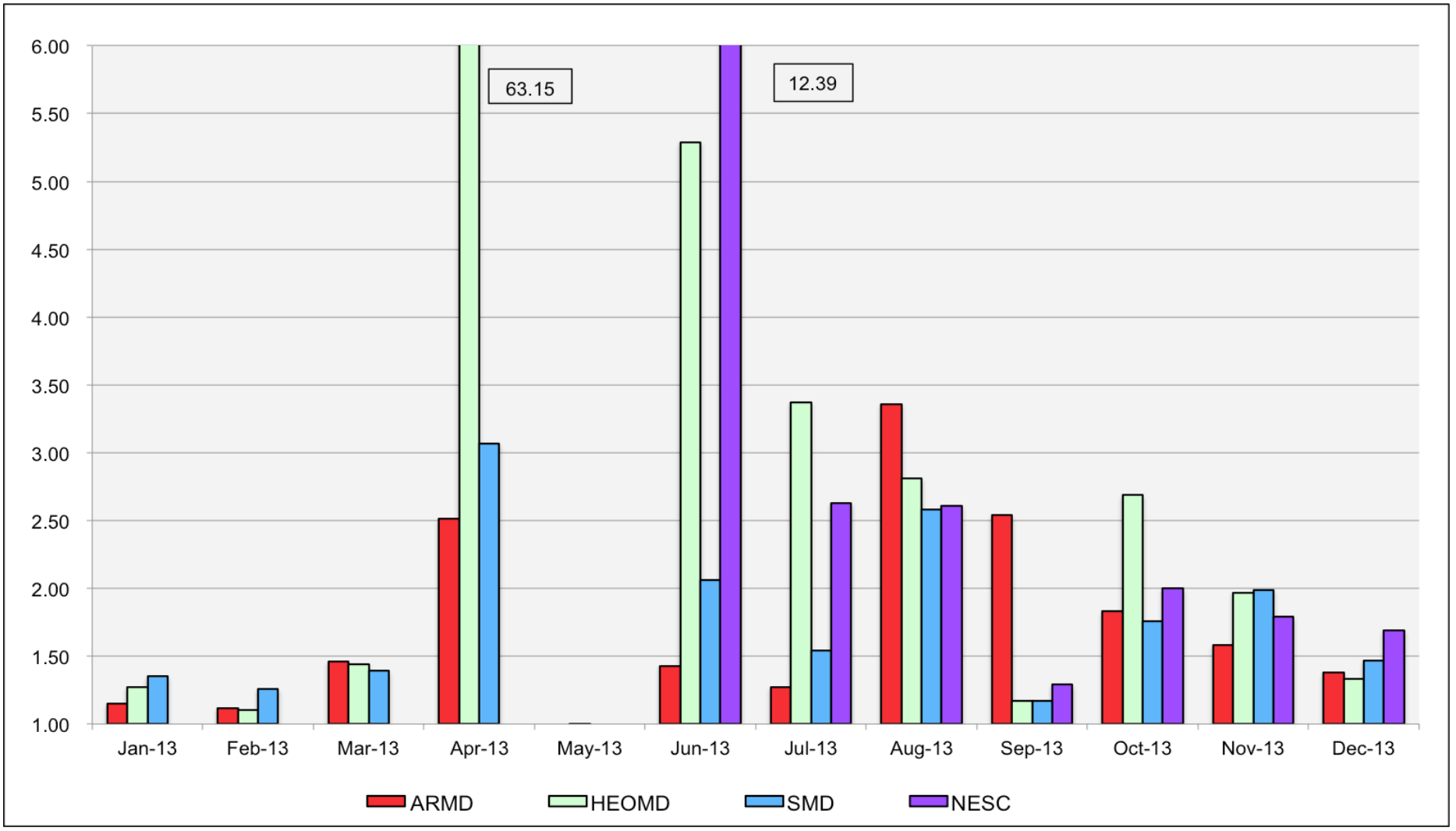
Pleiades:
Monthly Utilization by Size and Length



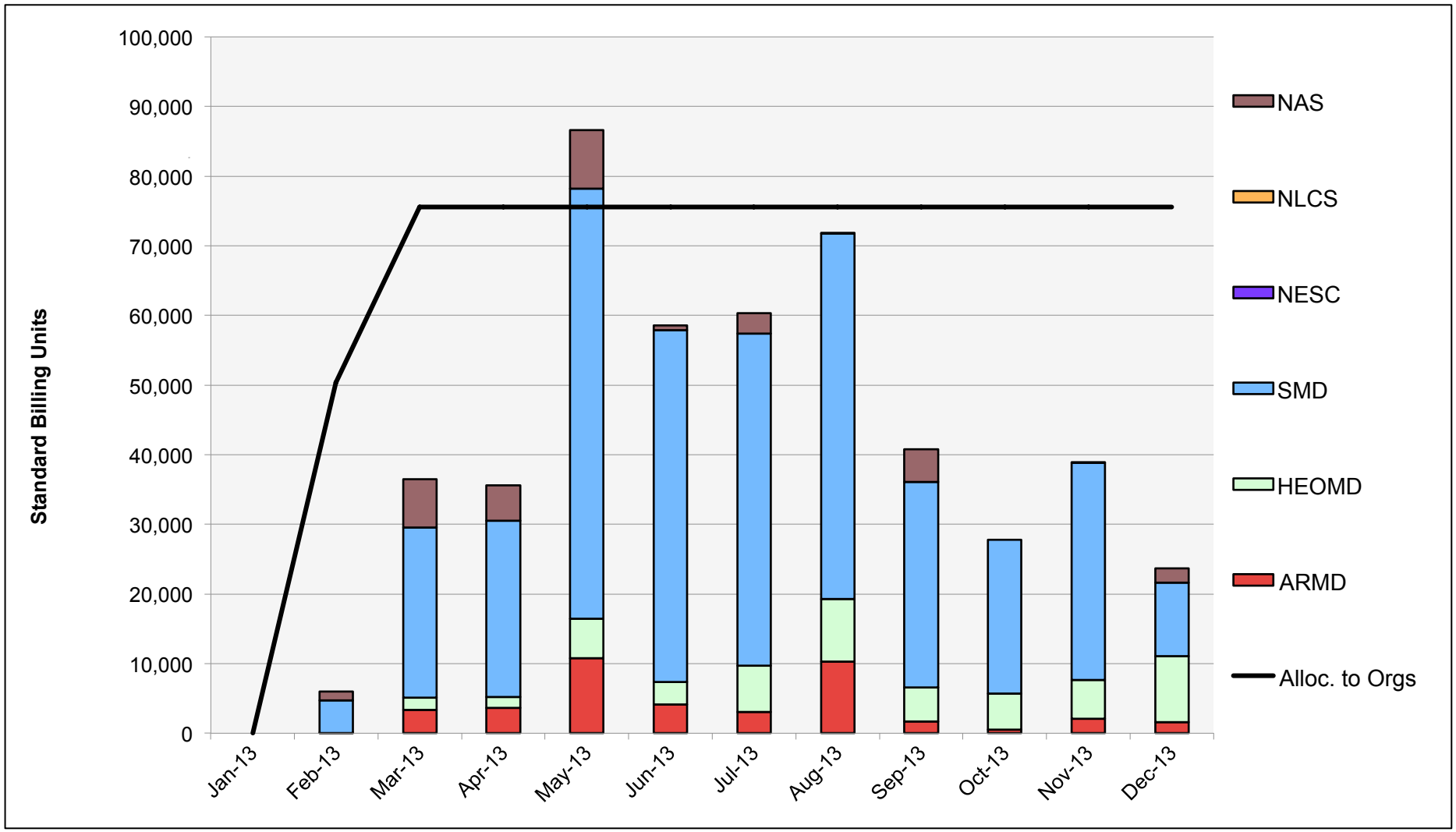
Pleiades:
Average Time to Clear All Jobs



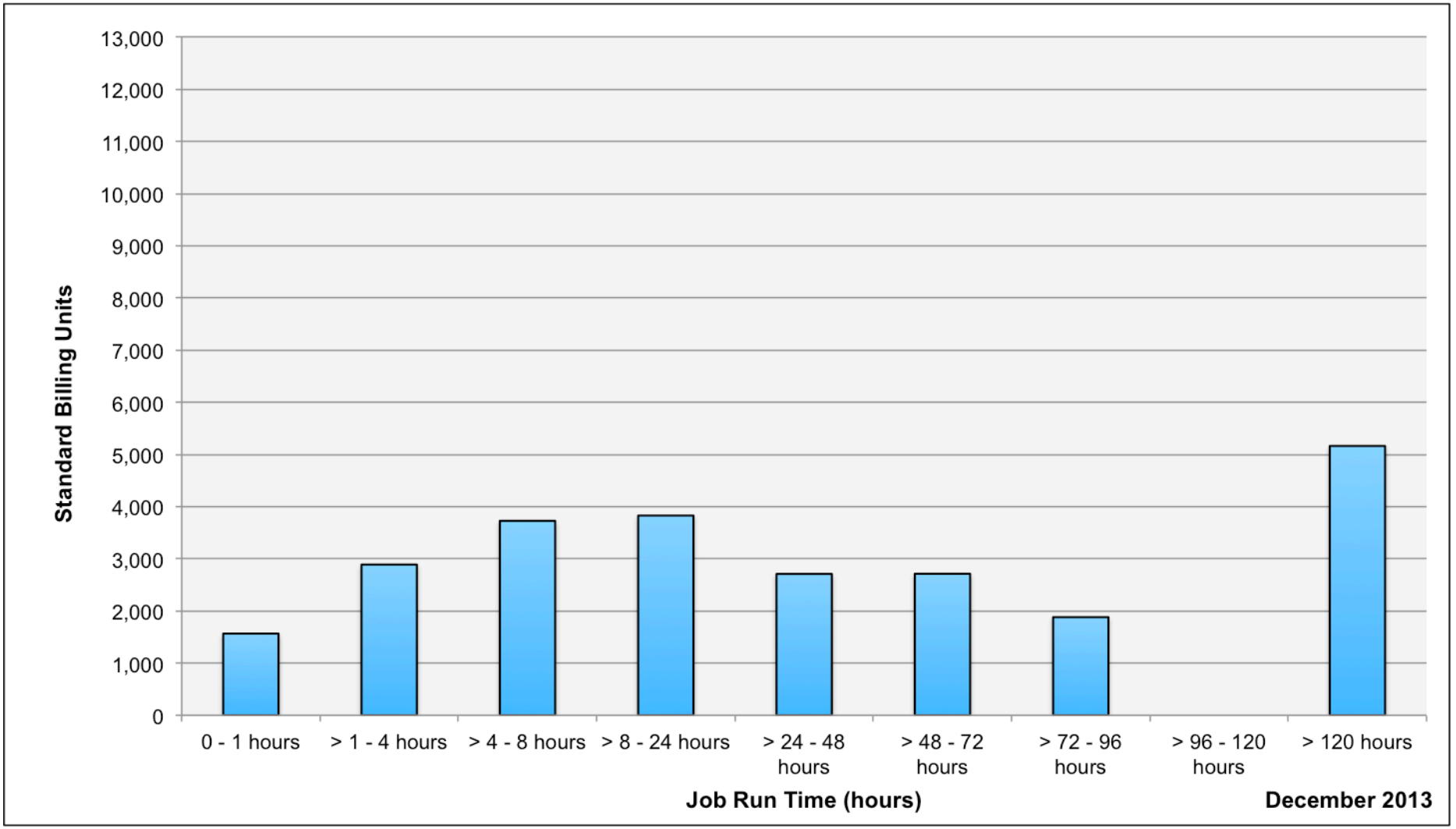
Pleiades:
Average Expansion Factor



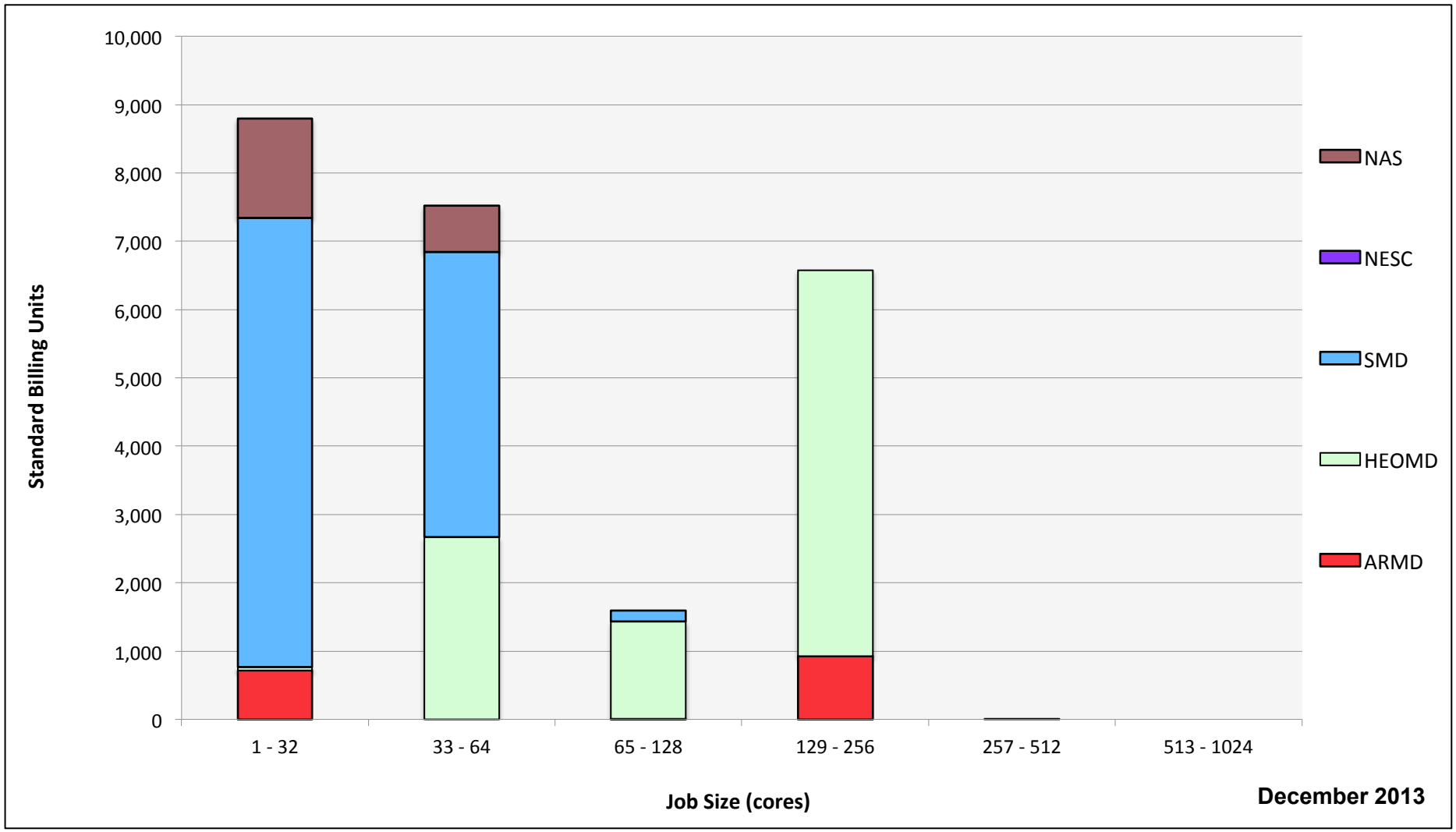
Endeavour:
SBUs Reported, Normalized to 30-Day Month



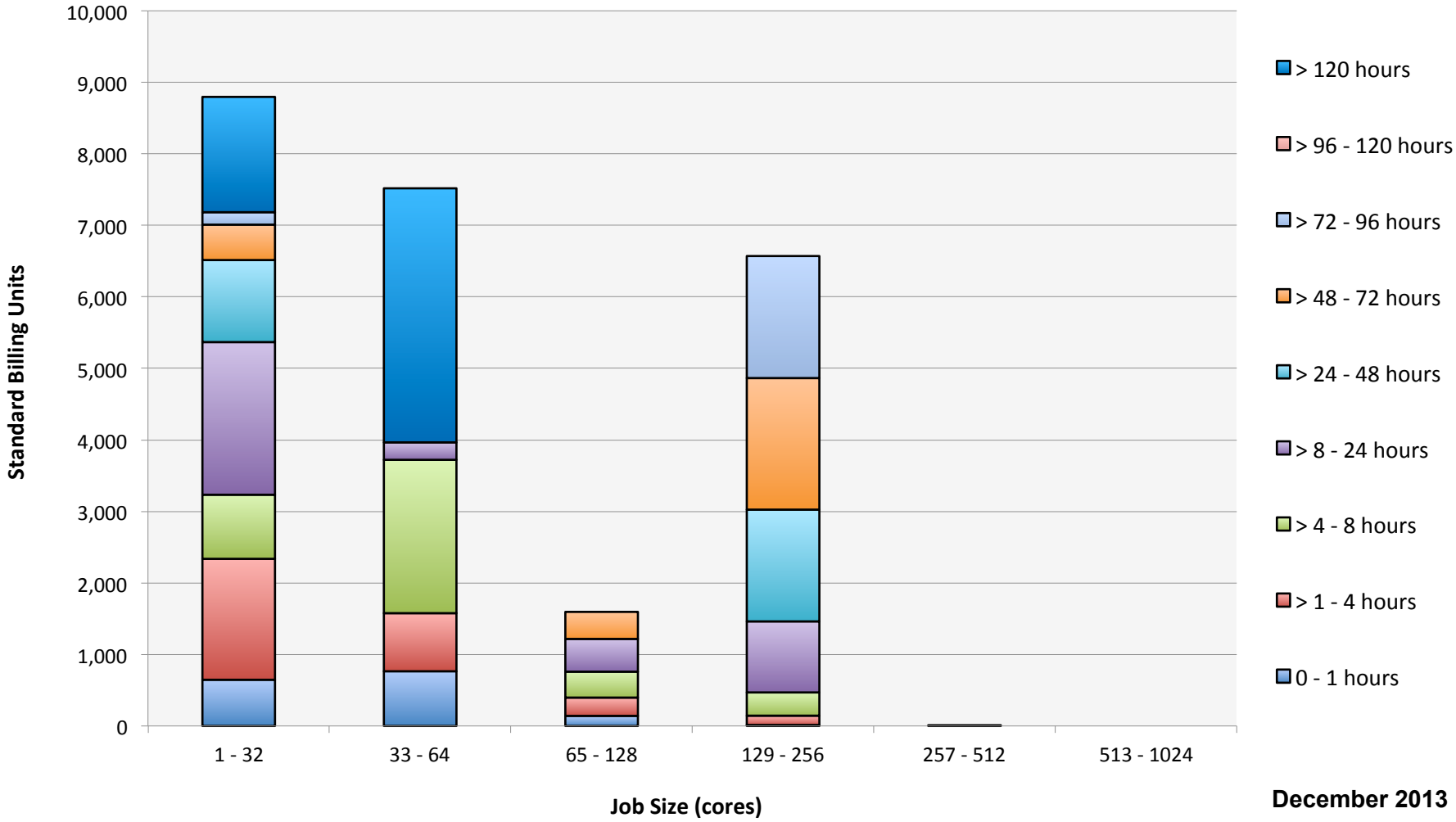
Endeavour:
Monthly Utilization by Job Length



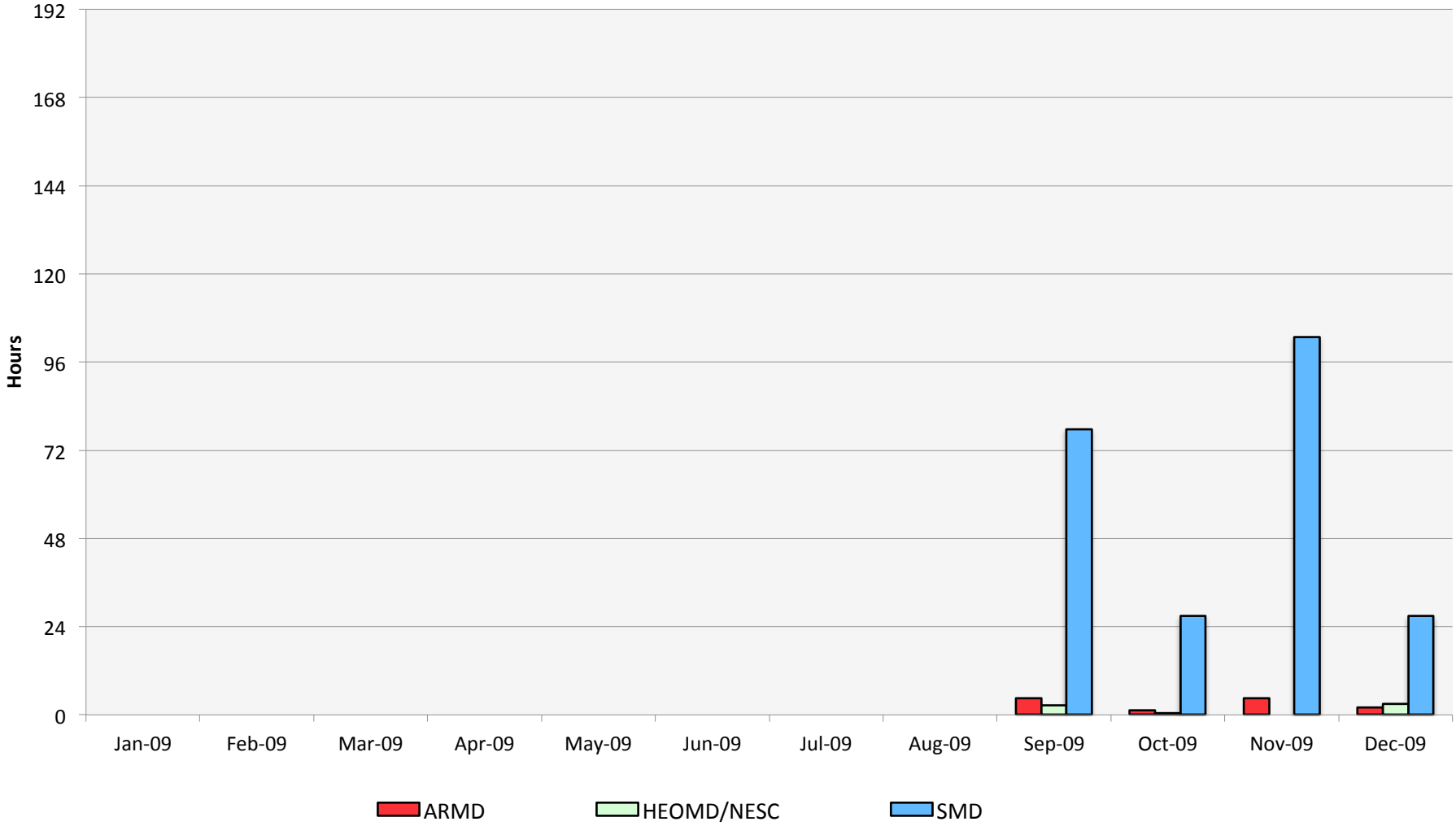
Endeavour:
Monthly Utilization by Size and Mission



Endeavour:
Monthly Utilization by Size and Length

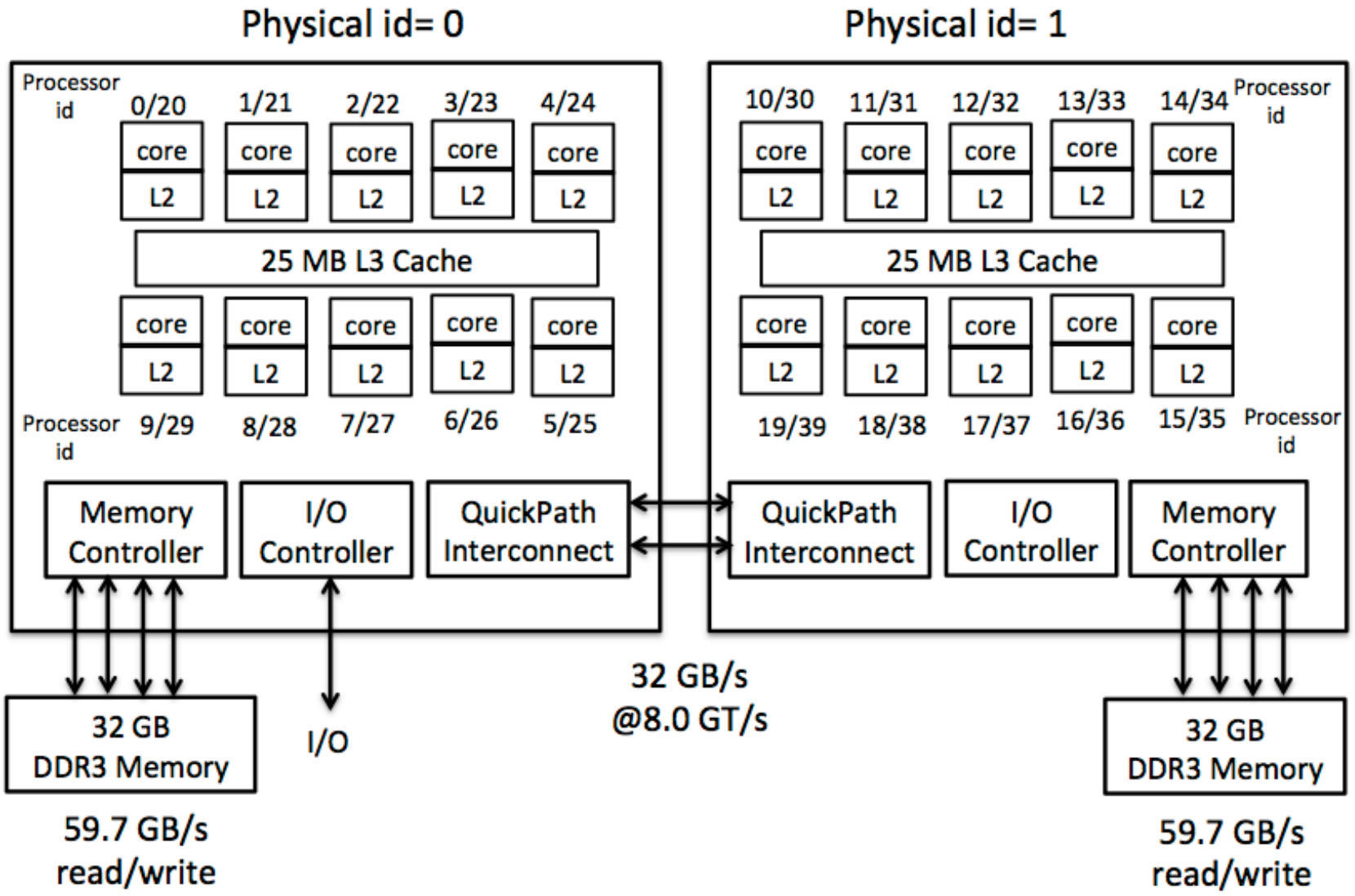


Endeavour:
Average Time to Clear All Jobs



Configuration of an Ivy Bridge-EP Node

Select image to return to presentation



Computing Time Comparison

Select image to return to presentation